A quadrature formula associated with a univariate quadratic spline quasi-interpolant

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Abstract

We study a new simple quadrature rule based on integrating a C^1 quadratic spline quasi-interpolant on a bounded interval. We give nodes and weights for uniform and non-uniform partitions. We also give error estimates for smooth functions and we compare this formula with Simpson's rule.

1 Introduction

We study a new simple quadrature formula (QF) based on integrating a C^1 quadratic spline quasi-interpolant (qi) on a bounded interval. It can be considered as the companion of Simpson's rule (as midpoint rule is the companion of trapezoidal rule) in the sense that the signs of errors for both QF are opposite in almost all examples. Here is an outline of the paper: in section 2, we recall the definition and main properties of the quadratic spline quasi-interpolants which are used. In section 3, we give the weights of the QF. In sections 4 and 5, we give estimates of the quadrature error for smooth functions in the cases of non-uniform and uniform partitions. In the latter case, we develop a more deeper study by using the associated Peano kernel and we compare our results to those of Simpson's rule. Finally, we illustrate our results with two numerical examples.
Regarding some recent papers close to ours, e.g. De Swardt & De Villiers [4], and Lampret [11], we use quadratic splines as the first one, however we do not consider interpolants, but quasi-interpolants (other QF based on spline quasi-interpolants are given in [18]) and our QF seems to have slightly better properties, at least than the Lacroix rule. The paper by Lampret is more oriented to the calculation of sums via the Euler-Maclaurin formula: it would be interesting to compare the performances our formula in this domain.

2 Univariate quadratic splines and discrete quasi-interpolants

Let $X = X_n = \{x_0, x_1, \ldots, x_n\}$ be a partition of a bounded interval $I = [a, b]$, with $x_0 = a$ and $x_n = b$. For $1 \le i \le n$, let $h_i = x_i - x_{i-1}$ be the length of the subinterval $I_i = [x_{i-1}, x_i]$ and let $\Gamma = \Gamma_n = \{0, 1, \ldots, n+1\}$. We denote by $\mathcal{S}_2(X)$ the $n+2$-dimensional space of C^1 quadratic splines on the partition X. A basis of this space is formed by the family of quadratic B-splines $\mathcal{B} = \{B_i,\ i \in \Gamma\}$, with triple knots $a = x_{-2} = x_{-1} = x_0$ and $b = x_n = x_{n+1} = x_{n+2}$. With these notations, the support of B_i is $[x_{i-2}, x_{i+1}]$ for all $i \in \Gamma$. Define the set of data sites (or Greville points):

$$\Theta_n = \{\theta_i = \frac{1}{2}(x_{i-1} + x_i)\ ; i \in \Gamma\}.$$

Note that $\theta_0 = x_0$ and $\theta_{n+1} = x_n$. In [16][17], we have proved the existence of a unique *discrete quasi-interpolant* (abbrev. dQI) of type

$$Qf = \sum_{i=0}^{n+1} \mu_i(f) B_i$$

whose discrete coefficient functionals are respectively $\mu_0(f) = f(x_0)$, $\mu_{n+1}(f) = f(x_n)$ and, for $1 \le i \le n$:

$$\mu_i(f) = a_i f(\theta_{i-1}) + b_i f(\theta_i) + c_i f(\theta_{i+1}),$$

which is exact on the space Π_2 of quadratic polynomials. Using the B-spline expansion of monomials and setting $e_k(x) = x^k$ for $k \ge 0$, we get (see e.g. [1],[12],[20]) :

$$e_0 = \sum_{i \in \Gamma} B_i, \quad e_1 = \sum_{i \in \Gamma} \theta_i B_i, \quad e_2 = \sum_{i \in \Gamma} x_{i-1} x_i B_i,$$

and writing the equations $Qe_k = e_k$ for $0 \le k \le 2$, we obtain:

$$a_i = -\frac{\sigma_i^2 \sigma'_{i+1}}{\sigma_i + \sigma'_{i+1}}, \quad b_i = 1 + \sigma_i \sigma'_{i+1}, \quad c_i = -\frac{\sigma_i (\sigma'_{i+1})^2}{\sigma_i + \sigma'_{i+1}},$$

with

$$\sigma_i = \frac{h_i}{h_{i-1} + h_i}, \quad \sigma'_i = 1 - \sigma_i = \frac{h_{i-1}}{h_{i-1} + h_i}.$$

We can now define the *fundamental functions* of $\mathcal{S}_2(X_n)$ associated with the quasi-interpolant Q:

$$\bar{B}_0 = B_0 + a_1 B_1, \quad \bar{B}_{n+1} = c_n B_n + B_{n+1},$$

and, for $1 \le i \le n$:

$$\tilde{B}_i = c_{i-1} B_{i-1} + b_i B_i + a_{i+1} B_{i+1}.$$

They allow to express Qf in the following shorter form:

$$Qf = \sum_{i \in \Gamma} f(\theta_i) \bar{B}_i,$$

and to show that the infinity norm of Q is equal to the Chebyshev norm of its Lebesgue function:

$$\Lambda_Q(x) = \sum_{i\in\Gamma} |\tilde{B}_i|.$$

In [20], Marsden proved the existence of a unique *Lagrange interpolant* $v \in \mathcal{S}_2(X)$ satisfying $v(\theta_i) = f(\theta_i)$ for $0 \le i \le n+1$. He also proved the following interesting result:

Theorem 1. The infinity norm of the Lagrange operator is uniformly bounded by 2, for any partition X of I.

There exists a similar result for the dQI Q defined above :

Theorem 2. For any partition X of I, the infinity norm of Q is uniformly bounded by 3. If the partition is uniform, one has $\|Q\|_\infty = \frac{305}{207} \approx 1.4734$.

proof : For the uniform case, see e.g. [17]. The first part of the proof is easy because we have

$$|\bar{B}_i| \le (|c_{i-1}| + b_i + |a_{i+1}|)B_i,$$

therefore, by summing on all indices, as B-splines sum to one :

$$\sum |\bar{B}_i| \le \max(|a_i| + b_i + |c_i|) = \max(1 + 2(|a_i| + |c_i|)) = \max(1 + 2\sigma_i\sigma_i') \le 3,$$

since $b_i = 1 - a_i - c_i = 1 + |a_i| + |c_i|$, and $\sigma_i, \sigma_i' \le 1$ $\square$

Remark. The results of this section are also valid when X contains some knots of multiplicity 2 or 3. Assume first that $\xi = x_p = x_{p+1}$ is a *double knot*, then Qf is only continuous at that point. Moreover as $h_{p+1} = 0$, we have $supp(B_p) = [x_{p-2}, \xi]$, $supp(B_{p+1}) = [\xi - h_p, \xi + h_{p+2}]$, $supp(B_{p+2}) = [\xi, x_{p+3}]$. Similarly, as $\sigma_{p+1} = 0$, we have $a_{p+1} = c_{p+1} = 0$ and $b_{p+1} = 1$, hence:

$$Qf = \sum_{i=0}^{p} \mu_i(f)B_i + f(\xi)B_{p+1} + \sum_{i=p+2}^{n+1} \mu_i(f)B_i.$$

Now, if $\eta = x_{q-1} = x_q = x_{q+1}$ is a *triple knot*, then $Q_2 f$ has a discontinuity at this point. Assume that f is itself discontinuous and admits left and right limits $f(\eta^-)$ and $f(\eta^+)$. Then as $h_q = h_{q+1} = 0$, we have $supp(B_q) = [\eta - h_{q-1}, \eta]$, with $B_q(\eta^-) = 1$ and $B_q(\eta^+) = 0$, while $supp(B_{q+1}) = [\eta, \eta + h_{q+2}]$, with $B_{q+1}(\eta^-) = 0$ and $B_{q+1}(\eta^+) = 1$. As $\sigma_q = \sigma_{q+1} = 0$, we get $a_q = a_{q+1} = c_q = c_{q+1} = 0$ and $b_q = b_{q+1} = 1$, hence:

$$Qf = \sum_{i=0s}^{q-1} \mu_i(f)B_i + f(\eta^-)B_q + f(\eta^+)B_{q+1} + \sum_{i=q+2}^{n+1} \mu_i(f)B_i.$$

Finally, from theorem 2 and standard arguments in approximation theory (see [5]) we deduce :

Theorem 3. There exists a constant $0 < C < 1$ such that for all $f \in W^{3,\infty}(I)$ and for all partitions of I, with $h = \max h_i$,

$$\|f - Qf\|_\infty \leq Ch^3 \|D^3 f\|_\infty.$$

3 Quadrature formula associated with Q

In this section, we compute the weights of the quadrature formula (abbr. QF) associated with the dQI Q, in the general case (non-uniform partition of the interval) and in the interesting particular case of a uniform partition.

3.1 Case of a non uniform partition

The QF associated with Q is of course obtained by integrating Qf:

$$\mathcal{I}_Q(f, I) = \int_a^b Qf = f(x_0) \int_a^b B_0 + \sum_{i=1}^n \mu_i(f) \int_a^b B_i + f(x_n) \int_a^b B_{n+1}.$$

We know that $w_i = \int_a^b B_i = \frac{1}{6}(h_{i-1} + 4h_i + h_{i+1})$ for $2 \leq i \leq n-1$ and

$$w_0 = \frac{1}{3}h_1,\ w_1 = \frac{1}{6}(3h_1 + h_2),\ w_n = \frac{1}{6}(h_{n-1} + 3h_n),\ w_{n+1} = \frac{1}{3}h_n.$$

Finally, we get the following QF:

$$\mathcal{I}_Q(f, I) = \sum_{i \in \Gamma} w_i \mu_i(f),$$

which can also be expressed in the classical form:

$$\mathcal{I}_Q(f, I) = \sum_{i \in \Gamma} \bar{w}_i f(\theta_i),$$

with $\bar{w}_0 = w_0 + a_1 w_1, \bar{w}_{n+1} = c_n w_n + w_{n+1}$, and for $1 \leq i \leq n$:

$$\bar{w}_i = \int_a^b \tilde{B}_i = c_{i-1} w_{i-1} + b_i w_i + a_{i+1} w_{i+1}.$$

The explicit expression of these weights is rather complicated. We only prove the following result :

Theorem 4.
1) For all partitions, the weights $\bar{w}_i$ satisfy $\sum_{i \in \Gamma} |\bar{w}_i| \leq 3(b-a)$.

2) More specifically, if there exists a $r > 0$ such that $\frac{1}{r} \leq \frac{h_{i+1}}{h_i} \leq r$ for all $1 \leq i \leq n-1$, then we have the more precise upper bound :

$$\sum_{i \in \Gamma} |\bar{w}_i| \leq (b-a)(1 + 2(\frac{r}{r+1})^2)$$

proof : $\sum_{i\in\Gamma} |\bar{w}_i| = \sum_{i\in\Gamma} |\int \bar{B}_i| \leq \int \sum_{i\in\Gamma} |\bar{B}_i| \leq \max(|a_i| + b_i + |c_i|) \int \sum_{i\in\Gamma} B_i \leq (b-a)\max(|a_i| + b_i + |c_i|) \leq 3(b-a)$, the last inequality being a consequence of theorem 2. In addition, when $\frac{1}{r} \leq \frac{h_{i+1}}{h_i} \leq r$ for all i, then we immediately deduce that $\frac{1}{r+1} \leq \sigma_i, \sigma'_i \leq \frac{r}{r+1}$ and $|a_i|+b_i+|c_i| = 1+2(|a_i|+|c_i|) = 1+2\sigma_i\sigma'_i \leq 1+2(\frac{r}{r+1})^2$, whence the result $\square$

Remark 1. As Q is exact on Π_2, we have $E_Q(f, I) = \mathcal{I}(f, I) - \mathcal{I}_Q(f, I) = 0$ for all $f \in \Pi_2$, therefore we can deduce that $E_Q(f, I) = O(h^3)$, with $h = \max h_i$ for smooth functions f (see section 5 below, theorem 5). However, when the partition X satisfy the *symmetry property* $x_i = x_{n-i}$, $0 \leq i \leq n$ (e.g. Chebyshev knots or, more generally, zeros of classical orthogonal polynomials in $I = [-1, 1]$, see e.g.[2][7][8][10]), then the weights are also symmetric and we also obtain $E_Q(e_3, I) = 0$. In that case, the error is a $O(h^4)$ for $f \in W^{4,\infty}(I)$, where $h = \max h_i$.

Remark 2. In general, the weights $\bar{w}_i$ are positive. However, they can be negative when the partition is strongly non-uniform. Take for example the following sequence of knots :

$$X = X_7 = \{-1, -0.9, -0.3, -0.2, 0.5, 0.6, 0.95, 1\}$$

whose associated sequence of steplengths is :

$$h_X = \{0.1, 0.6, 0.1, 0.7, 0.1, 0.35, 0.05\}$$

Here we have $r = 7$, i.e. $\frac{1}{7} \leq \frac{h_{i+1}}{h_i} \leq 7$ for all i, and theorem 4 gives the upper bound $\sum_{i\in\Gamma} |\bar{w}_i| \leq \frac{81}{16} \approx 5.06$. The sequence of weights is the following :

$$\bar{w} = \{.0146, .0122, .7463, .-.0622, .8780, -.0257, .4287, .0007, .0074\}$$

We observe that the weights $\bar{w}_3$ and $\bar{w}_5$ are negative : however, their absolute values are small. Moreover, we have $\sum_{i\in\Gamma} |\bar{w}_i| = 2.17 < 5.06$.

3.2 Case of a uniform partition

Assume that $n \geq 5$ (in order to avoid boundary effects) and that the partition X_n is uniform: $h_i = h = \frac{b-a}{n}$ for $1 \leq i \leq n$. In that case, the weights can be computed once for all and we obtain, by setting $f_j = f(\theta_j), j \in \Gamma$ (see e.g. [16][17][18]):

$$\mathcal{I}_Q(f, I) = h\,[\,\frac{1}{9}(f_0 + f_{n+1}) + \frac{7}{8}(f_1 + f_n) + \frac{73}{72}(f_2 + f_{n-1}) + \sum_{i=3}^{n-2} f_i\,].$$

As for some Newton-Cotes QF, this QF has a better degree of precision:

Theorem 4. The QF associated with the dQI Q on a uniform partition of I is exact on the space Π_3 of cubic polynomials. Therefore $E(f,I)=O(h^4)$ for f smooth enough.

proof : This is due to the symmetry of weights and nodes with respect to the midpoint of I. $\square$

4 Error estimate on a non-uniform partition

As we have already seen in section 4, $E_Q(f,I)=\mathcal{I}(f,I)-\mathcal{I}_Q(f,I)=O(h^3)$ when the partition X of $I=[a,b]$ is non-uniform, with $h=\max_{1\le i\le n} h_i$. In this section, we give more specific results when $f\in W^{3,\infty}(I)$. From theorem 3, we immediately deduce:

Theorem 5. There exists a constant $0<C_3<b-a$ such that for all $f\in W^{3,\infty}(I)$ and for all partitions X of I, with $h=\max_{1\le i\le n} h_i$:

$$|E_Q(f,I)|\le C_3 h^3\|D^3 f\|_\infty.$$

proof : we know (theorem 3) that there exists a constant $0<C<1$ such that $\|f-Qf\|_\infty\le Ch^3\|D^3f\|_\infty$. As $E_Q(f,I)=\mathcal{I}(f-Qf)$, we can write:

$$|E_Q(f,I)|\le\int_a^b|f-Qf|\le(b-a)\,Ch^3\|D^3f\|_\infty.$$

Therefore we get the result with $C_3=(b-a)C$. $\square$

5 Error estimate on a uniform partition

Assume that the partition X_n is uniform ($h_i=h=\frac{b-a}{n}$ for $1\le i\le n$) and that $f\in W^{4,\infty}(I)$. As $\mathcal{I}_Q(f,I)$ is exact on Π_3, the Peano kernel theorem (se e.g. [2], chapter III) gives:

$$E_Q(f,I)=\frac{1}{6}\int_a^b K(t)D^4f(t)dt,$$

where

$$K(t)=\int_a^b[(x-t)_+^3-Q(.-t)_+^3]dx,$$

and

$$Q(.-t)_+^3=\sum_{i\in\Gamma}(\theta_i-t)_+^3\bar{B}_i.$$

As $\int_a^b (x-t)_+^3 dx = \int_t^b (x-t)^3 dx = \frac{1}{4}(b-t)^4$, we obtain:

$$K(t) = \frac{1}{4}(b-t)^4 - \sum_{i\in\Gamma} \tilde{w}_i(\theta_i - t)_+^3.$$

We see immediately that $K(a) = K(b) = 0$. First, it is clear that $K(b) = 0$ since $(\theta_i - b)_+^3 = 0$ for all $i \in \Gamma$. Second, let $p(x) = (x-a)^3$, then $\mathcal{I}(p) = \frac{1}{4}(b-a)^4 = \mathcal{I}_Q(p) = \sum_{i\in\Gamma} \tilde{w}_i p(\theta_i)$ since $p \in \Pi_3$, therefore $K(a) = \frac{1}{4}(b-a)^4 - \sum_{i\in\Gamma} \tilde{w}_i(\theta_i - a)^3 = 0$.

5.1 Sign structure of the Peano kernel

For the sake of simplicity, we now assume that $I = [0,1]$, then $h = \frac{1}{n}$ and $\theta_i = (i - \frac{1}{2})\, h$ for $1 \le i \le n$, with $\theta_0 = 0$ and $\theta_{n+1} = 1$. Therefore we have:

$$K(t) = \frac{1}{4}(1-t)^4 - h\,[\frac{7}{8}\left(\frac{h}{2} - t\right)_+^3 + \frac{73}{72}\left(\frac{3h}{2} - t\right)_+^3 + \frac{73}{72}\left((n - \frac{3}{2})h - t\right)_+^3$$

$$+\frac{7}{8}\left((n - \frac{1}{2})h - t\right)_+^3 + \frac{1}{9}(1-s)_+^3] + \sum_{i=3}^{n-2}\left((i - \frac{1}{2})h - t\right)_+^3.$$

It is not difficult to prove that $K(1-t) = K(t)$. Actually, setting

$$K(t) = \frac{1}{4}(1-t)^4 - \sum_{i=0}^{n+1} w_i(\theta_i - t)_+^3$$

and using the symmetry of nodes and weights, we get

$$K(1-t) = \frac{1}{4}t^4 - \sum_{i=0}^{n+1} w_i(t - \theta_i)_+^3.$$

Now, we observe that $(\theta_i - t)_+^3 - (t - \theta_i)_+^3 = (\theta_i - t)^3$ and that the cubic polynomial $p(s) = (s-t)^3$ is exactly integrated by the QF, hence:

$$\int_0^1 p(s)ds = \sum_{i=0}^{n+1} w_i p(\theta_i) \Longleftrightarrow \frac{1}{4}[(1-t)^4 - t^4] - \sum_{i=0}^{n+1} w_i(\theta_i - t)^3 = 0.$$

The above properties imply that

$$K(t) - K(1-t) = \frac{1}{4}[(1-t)^4 - t^4] - \sum_{i=0}^{n+1} w_i[(\theta_i - t)_+^3 - (t - \theta_i)_+^3] = 0.$$

In the interval $I_1 = [0, \theta_1] = [0, \frac{h}{2}]$, we have:

$$K(t) = K_1(t) = \frac{1}{4}t^4 - \frac{h}{9}t^3 = \frac{1}{4}t^3\left(t - \frac{4h}{9}\right), \quad K_1'(t) = t^2\left(t - \frac{h}{3}\right).$$

Therefore, it is clear that K_1 has a minimum $K_1(\frac{h}{3}) = -\frac{h^4}{972}$, that $K_1(\frac{4h}{9}) = 0$ and $K_1(\theta_1) = K_1(\frac{h}{2}) = \frac{h^4}{576}$. Moreover $K_1'(\frac{h}{2}) = \frac{h^3}{24}$.

In the interval $I_2 = [\theta_1, \theta_2] = [\frac{h}{2}, \frac{3h}{2}]$, we have:

$$K(t) = K_2(t) = K_1(t) - \frac{7h}{8}\left(t - \frac{h}{2}\right)^3, \quad K_2'(t) = K_1'(t) - \frac{21h}{8}\left(t - \frac{h}{2}\right)^2.$$

As $K_1'(\theta_2) = K_1'(\frac{3h}{2}) = \frac{21h^3}{8}$, we see that $K_2'(\theta_2) = 0$, therefore we can factorize:

$$K_2'(t) = \left(t - \frac{3h}{2}\right)\left(t^2 - \frac{35h}{24}t + \frac{7h^2}{16}\right),$$

and we deduce that $K_2' = 0$ for $t = \frac{3h}{2}$ and $t = \bar{t} = \frac{35+\sqrt{217}}{48}h \approx 1.036h$. Therefore K_2 has a maximum at the latter point and

$$K_2(\bar{t}) \approx 0.03h^4 \leq \frac{h^4}{32},$$

moreover, we have $K_2(\theta_1) = K_1(\theta_1) = \frac{h^4}{576}$, $K_2(\theta_2) = \frac{h^4}{64}$, and we can factorize:

$$K_2(t) - \frac{h^4}{64} = \frac{1}{8}\left(t - \frac{3h}{2}\right)^2\left(t^2 - \frac{17h}{18}t + \frac{h^2}{6}\right).$$

In the interval $I_3 = [\theta_2, \theta_3] = [\frac{3h}{2}, \frac{5h}{2}]$, we have:

$$K(t) = K_3(t) = K_2(t) - \frac{73h}{72}\left(t - \frac{3h}{2}\right)^3, \quad K_3'(t) = K_2'(t) - \frac{73h}{24}\left(t - \frac{3h}{2}\right)^2.$$

As $K_2'(\theta_2) = 0$, we see that $K_3'(\theta_2) = 0$, therefore we can factorize:

$$K_3'(t) = \left(t - \frac{3h}{2}\right)\left(t^2 - \frac{9h}{2}t + 5h^2\right) = \left(t - \frac{3h}{2}\right)(t - 2h)\left(t - \frac{5h}{2}\right),$$

and we deduce that K_3 has one maximum and two minima:

$$K_3(2h) = \frac{h^4}{32}, \quad K_3\left(\frac{3h}{2}\right) = K_3\left(\frac{5h}{2}\right) = \frac{h^4}{64}.$$

Finally, we also obtain the factorization:

$$K_3(t) - \frac{h^4}{64} = \frac{1}{4}\left(t - \frac{3h}{2}\right)^2\left(t - \frac{5h}{2}\right)^2.$$

Now, in the intervals $I_i = [\theta_{i-1}, \theta_i] = [(i - \frac{3}{2})h, (i - \frac{1}{2})h]$, for $4 \leq i \leq n-2$, if we assume that

$$K_i(t) - \frac{h^4}{64} = \frac{1}{4}\left(t - (i - \frac{3}{2})h\right)^2\left(t - (i - \frac{1}{2})h\right)^2,$$

as we have, by definition

$$K_{i+1}(t) = K_i(t) - \left(t - (i - \frac{1}{2})h\right)^3,$$

we immediately obtain

$$\begin{aligned} K_{i+1}(t) - \frac{h^4}{64} &= \frac{1}{4}\left(t-(i-\frac{1}{2})h\right)^2 \left[\left(t-(i-\frac{3}{2})h\right)^2 - 4\left(t-(i-\frac{1}{2})h\right)\right] \\ &= \frac{1}{4}\left(t-(i-\frac{1}{2})h\right)^2 \frac{1}{4}\left(t-(i+\frac{1}{2})h\right)^2. \end{aligned}$$

Therefore, we deduce that, in the interval I_i, $K = K_i$ has one maximum and two minima

$$K_i((i-1)h) = \frac{h^4}{32}, \quad K_i\left((i-\frac{3}{2})h\right) = K_i\left((i-\frac{1}{2})h\right) = \frac{h^4}{64}.$$

In the three last subintervals $I_{n-1} = [1-\frac{5h}{2}, 1-\frac{3h}{2}], I_n = [1-\frac{3h}{2}, 1-\frac{h}{2}]$ and $I_{n+1} = [1-\frac{h}{2}, 1]$, the behaviour of K is symmetrical of that one in the three first subintervals. To sum up, we obtain

Theorem 6. The Peano kernel K is negative in the two small subintervals $J_1 = [0, \frac{4h}{9}]$ and $J_3 = [1-\frac{4h}{9}, 1]$ and positive in the subinterval $J_2 = [\frac{4h}{9}, 1-\frac{4h}{9}]$.

5.2 Error estimate for the quadrature formula

Let $f \in C^4(I)$ be a given function, then from

$$E_Q(f, I) = \frac{1}{6}\int_0^1 K(t)D^4 f(t)dt$$

and theorem 6, we deduce:

Theorem 7. For any function $f \in C^4(I)$, there exists two points $c, \bar{c} \in I$ such that

$$E_Q(f, I) = \frac{23}{5760}h^4 D^4 f(c) - \frac{1}{192}h^5 D^4 f(\bar{c}).$$

proof : From the mean value theorem, we know that there exists $c_1 \in J_1, c_2 \in J_2$ and $c_3 \in J_3$ such that

$$E_Q(f, I) = \frac{1}{6}\left[D^4 f(c_1)\int_0^{\frac{4h}{9}} K(t)dt + D^4 f(c_2)\int_{\frac{4h}{9}}^{1-\frac{4h}{9}} K(t)dt + D^4 f(c_3)\int_{1-\frac{4h}{9}}^1 K(t)dt\right].$$

We compute successively

$$\int_0^{\frac{4h}{9}} K(t)dt = \frac{1}{4}\int_0^{\frac{4h}{9}} t^3\left(t - \frac{4h}{9}\right)dt = -\frac{64h^5}{295245},$$

$$\int_{\frac{4h}{9}}^{\frac{h}{2}} K(t)dt = \int_{\frac{4h}{9}}^{\frac{h}{2}} t^3 \left(t - \frac{4h}{9}\right) dt = \frac{1631h^5}{37791360},$$

$$\int_{\frac{h}{2}}^{\frac{3h}{2}} K(t)dt = \frac{59h^5}{2880},$$

and for $2 \leq i \leq n-2$:

$$\int_{(i-\frac{1}{2})h}^{(i+\frac{1}{2})h} K(t)dt = \frac{23h^5}{960}.$$

Then, using $nh = 1$ and setting $\gamma_1 = \frac{64}{295245}, \gamma_2 = \frac{23}{960}, \gamma_3 = \frac{291149}{9447840}$, we obtain successively:

$$\int_{\frac{3}{2}h}^{1-\frac{5}{2}h} K(t)dt = (n-3)\frac{23h^5}{960} = \frac{23h^4}{960} - \frac{23h^5}{320}.$$

$$\int_{J_2} K(t)dt = \gamma_2 h^4 - h^5 \left(2 \times \frac{1631}{37791360} + 2 \times \frac{59}{2880} - \frac{23}{320}\right) = \gamma_2 h^4 - \gamma_3 h^5,$$

$$\int_{J_1} K(t)dt = \int_{J_3} K(t)dt = -\gamma_1 h^5.$$

Now, setting $\bar{\gamma}_j = \gamma_j/6$ for $1 \leq j \leq 3$, we have:

$$E_Q(f,I) = \frac{1}{6}\int_0^1 K(t)D^4 f(t)dt = \bar{\gamma}_2 h^4 D^4 f(c_2) - h^5 \left[\bar{\gamma}_1 D^4 f(c_1) + \bar{\gamma}_3 D^4 f(c_2) + \bar{\gamma}_1 D^4 f(c_3)\right].$$

Finally, setting $\bar{\gamma}_4 = 2\bar{\gamma}_1 + \bar{\gamma}_3$, the mean-value theorem implies that there exists a point $c_4 \in I$ such that

$$E_Q(f,I) = \bar{\gamma}_2 h^4 D^4 f(c_2) - \bar{\gamma}_4 h^5 D^4 f(c_4),$$

with $\bar{\gamma}_2 = \frac{23}{5760}$ and $\bar{\gamma}_4 = \frac{1}{192}$. □

Remark. For n large enough, one can write

$$E_Q(f,I) = \frac{23}{5760} h^4 D^4 f(c) + O(h^5),$$

therefore, the main part of the error is contained in the first term.

5.3 Comparison with composite Simpson's rule and extrapolation

Let us compare the above error with the quadrature error $E_S(f,I) = \mathcal{I}(f,I) - \mathcal{I}_S(f,I)$ of composite Simpson's rule. Taking $n = 2m$ even, the latter is based on the $n+1$ points $\{x_j, 0 \leq j \leq n\}$, while our QF is based on the set $\{\theta_i, 0 \leq i \leq n+1\}$ which has $n+2$ points. It is well known (see e.g. [2][3][6][10]) that for any function $f \in C^4(I)$, there exists a point $d \in I$ such that:

$$E_S(f,I) = -\frac{1}{180} h^4 D^4 f(d).$$

Therefore, *when $D^4 f$ is of one sign* over the interval I, the quadrature errors are of *opposite signs*, i.e. the two formulas give *lower and upper estimates* of the value of the integral.

Remark: as shown by numerical examples below, the following linear combination obtained by extrapolation

$$\mathcal{I}_{QS}(f,I) = \frac{1}{55}(32\mathcal{I}_Q(f,I) + 23\mathcal{I}_S(f,I))$$

gives a still better approximation, with an order $O(h^5)$ (notice the nice symmetry of weights).

6 Numerical results

For the two following functions f_1, f_2 and f_3 (other examples are given in [18]), we give the quadrature errors $E_Q(f)$, $E_S(f)$ and $E_{QS}(f)$ in terms of the number n of subintervals:

Example 1:

$\mathcal{I}(f_1,I) = \int_0^1 16x^{3/2} sin\,(x^2)\,dx = 3.2523064663781227544.$

n	$E_Q(f_1)$	$E_S(f_1)$	$E_{QS}(f_1)$
64	$-.86(-7)$	$1.23(-7)$	$1.13(-9)$
128	$-.54(-8)$	$.76(-8)$	$.16(-10)$
256	$-.34(-9)$	$.47(-9)$	$-.40(-12)$
512	$-.21(-10)$	$.29(-10)$	$-.52(-13)$
1024	$-.13(-11)$	$.18(-11)$	$-.33(-14)$

Example 2:

$$\mathcal{I}(f_2,I) = \int_0^1 \left(\frac{1}{(x-0.3)^2+0.01} + \frac{0.8}{(x-0.7)^2+0.04} \right) dx = 35.880612010038328566$$

n	$E_Q(f_2)$	$E_S(f_2)$	$E_{QS}(f_2)$
64	$-.19(-5)$	$.23(-5)$	$-.14(-6)$
128	$-.11(-6)$	$.14(-6)$	$-.37(-8)$
256	$-.67(-8)$	$.90(-8)$	$-.11(-9)$
512	$-.41(-9)$	$.56(-9)$	$-.35(-11)$
1024	$-.25(-10)$	$.35(-10)$	$-.11(-12)$

Example 3 :

$$\mathcal{I}(f_3, I) = \int_{-1}^{1} \frac{1}{1+16x^2}\,dx = 0.66290883183401623252961 95.$$

n	$E_Q(f_2)$	$E_S(f_2)$	$E_{QS}(f_2)$
256	$-.33(-10)$	$.46(-10)$	$-.44(-12)$
512	$-.21(-11)$	$.28(-11)$	$-.13(-13)$
1024	$-.13(-12)$	$.18(-12)$	$-.42(-15)$
2048	$-.80(-14)$	$.11(-13)$	$-.13(-16)$
4096	$-.50(-15)$	$.69(-15)$	$-.41(-18)$

Note that the signs of errors are opposite when h is small enough.

Abbreviations of editors in references:
AP=Academic Press, London, New-York. BV=Birkhäuser Verlag, Basel.
Bl=Blaisdell, Waltham. CUP=Cambridge University Press.
Dov=Dover Publ., New-York. JWS=John Wiley & Sons, New-York.
IRMAR=Institut de Recherche Mathématique de Rennes.
SIAM=Society for Industrial and Applied Mathematics, Philadelphia.
SV=Springer-Verlag, Berlin, New-York.

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